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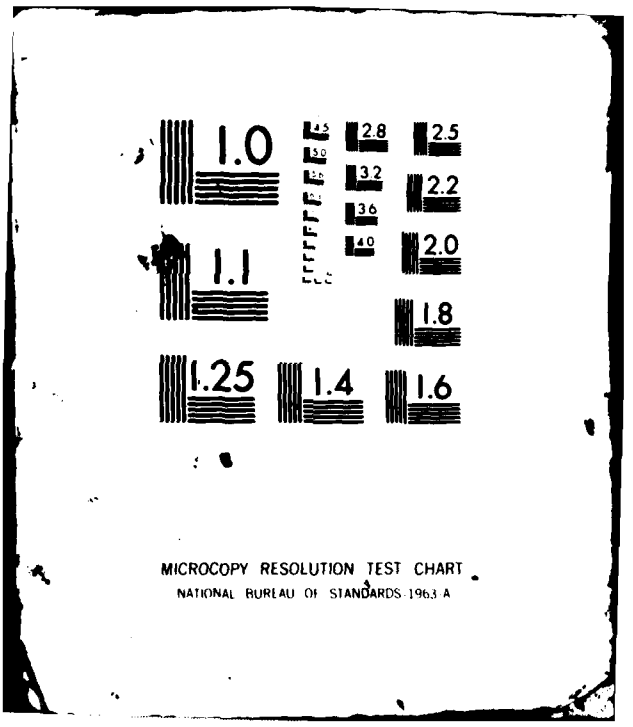
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STRUCTURE AND INTERACTIONS IN ORGANIC AGGREGATES

FINAL REPORT

to the

U.S. Army Research Office

Grant no. DAAG29-79-G-0032

submitted by:

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The research program we have pursued during the past three years of ARO support has been focused on the physical features of organic dimers and higher order aggregates as revealed through the triplet state properties of these complexes. The overall aim of the research effort was to elucidate the structural features of aromatic organic aggregate systems and the interactions which stabilize them, with a view toward understanding the nature of aggregation as it occurs in model systems of importance in photochemistry and photobiology.

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The research program we have pursued during the past three years of ARO support has been focused on the physical features of organic dimers and higher order aggregates as revealed through the triplet state properties of these complexes. The overall aim of the research effort was to elucidate the structural features of aromatic organic aggregate systems and the interactions which stabilize them, with a view toward understanding the nature of aggregation as it occurs in model systems of importance in photochemistry and photobiology.

Our approach utilized the photoexcited triplet state of the complexes as a (nondestructive) paramagnetic probe into the physical makeup of these systems, using optically detected magnetic resonance (ODMR) spectroscopy, a technique developed and refined in our laboratory under ARO support over the past several years, as the principal experimental tool. ODMR has allowed the investigation of a wide variety of aggregates formed from large, multi-ring aromatic organic molecules, through its combination of the sensitivity of an optical experiment with the resolution of magnetic resonance.

In overview, our research accomplishments during the past period of ARO support have been mainly in the areas of [illegible]standing: (1) the ligand-bound dimeric and oligomeric complexes of the chlorophylls, systems whose (weak) intermolecular interactions are determined more by ligand-chlorophyll interactions than by direct pigment-pigment interactions; and (2) the (strongly interacting) intramolecular dimer systems, as represented by the biquinoline molecule, a dimer of two covalently attached quinoline ring units. These systems have provided a wide-ranging test of the application of the triplet exciton approach to the description of organic dimers, with

results which both indicate the strengths and define the limitations of such a dimer description, providing a basis for the approach to evaluation of organic aggregate structure in aromatic ring systems.

The specific research accomplishments in the above areas during the past period under ARO support are detailed in the following publications:

R.H. Clarke, D.R. Hobart and W.R. Leenstra
The Triplet State of the Chlorophyll Dimer
J. Am. Chem. Soc., 101, 2416 (1979).

R.P.H. Kooyman, T.J. Schaafsma, G. Jansen, R.H. Clarke
D.R. Hobart and W.R. Leenstra
A Comparative Study of Dimerization of Chlorophylls and Pheophytins by Fluorescence and ODMR
Chem. Phys. Letters, 68, 65 (1979)

R.H. Clarke, S.P. Jagannathan and W.R. Leenstra
Optical-Microwave Double Resonance Spectroscopy of in vivo Chlorophyll
Lasers in Photomedicine and Photobiology, R. Pratesi and D.A. Sacchi, eds. (Springer-Verlag, Berlin, 1980), p. 171.

R.F. Clark and R.H. Clarke
Electron Delocalization in the Lowest Triplet State of the Covalently-Linked Pyrochlorophyllide a Dimer
J. Chem. Phys., 73, 5386 (1980)

R.H. Clarke, P. Mitra and K. Vinodgopal
Phosphorescence and Zero-Field ODMR of Biquinoline
Chem. Phys. Letters, 76, 237 (1980)

R.H. Clarke, S.P. Jagannathan and W.R. Leenstra
Optical-Microwave Double Resonance of in vivo Chlorophyll
Photochem. Photobiol., 32, 805 (1980)

D.R. Hobart
The Triplet State of the Chlorophyll Dimer
Ph.D. Thesis, Boston University, 1981

R.H. Clarke
The Chlorophyll Triplet State and the Structure of Chlorophyll Aggregates
Light Reactions in Photosynthesis, F. Fong, ed., (Springer-Verlag, Berlin, 1982), in press

R.H. Clarke (editor)
Triplet State ODMR Spectroscopy: Techniques and Applications to Biophysical Systems
Wiley-Interscience, New York, N.Y. 1982

R.H. Clarke and S.P. Jagannathan
Optically Detected Zero-Field Triplet State Spectroscopy of *in vivo* Chlorophyll
Proceedings of the Fifth International Congress on Photosynthesis, G.A. Akoyunoglou, ed., in press

and in the following papers presented at major international meetings:

Europhysics Conference on Lasers in Photomedicine and Photobiology, Florence, Italy, September 3-7, 1979 (invited talk)

Fourth Grodon Research Conference on Magnetic Resonance in Medicine and Biology
Tilton, New Hampshire, August 10-15, 1980 (invited talk)

Fifth International Congress on Photosynthesis
Kallithea, Greece, September 7-13, 1980

Symposium on Spectroscopy and Dynamics
Philadelphia, PA, April 8-10, 1981 (invited talk)

Personnel involved in the research program included:

R.H. Clarke - principal investigator

W.R. Leenstra - postdoctoral research associate, 1979-81

D.R. Graham - postdoctoral research associate, 1981

D.R. Hobart - graduate research assistant (Ph.D. received, 1981)

P. Mitra - graduate research assistant (Ph.D. received, 1982)

K. Vinodgopal - graduate research assistant (Ph.D. candidate)

E. Hanlon - graduate research assistant (Ph.D. candidate)